Supporting Information

Water-Soluble, Redox-Active Organometallic Calcium Chelators

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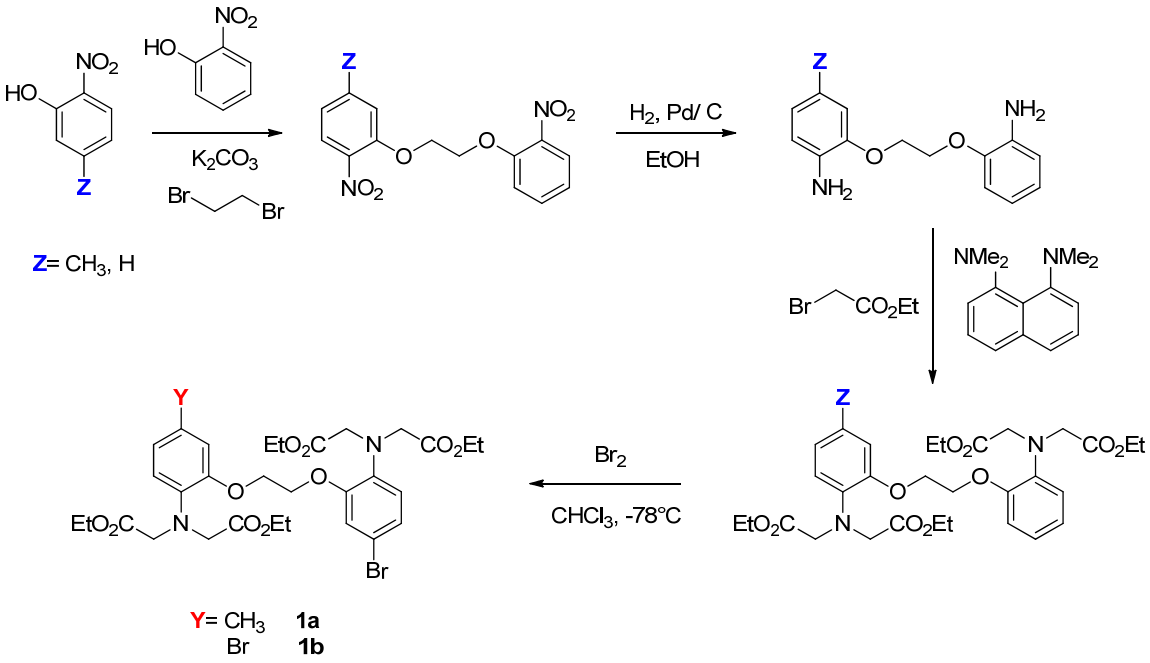
I- Synthesis of 5-bromo-5'-Methyl-BAPTA ethyl ester (1a) and 5,5'-dibromo-BAPTA ethyl ester (1b).

(BAPTA = 1,2-bis(2aminophenoxy)-ethane- N,N,N',N'-tetraacetic acid). For synthesis details of ***1a-b*** *see* [1-2]



Scheme S1: Synthesis of the bromo-BAPTA tetra-ester **1a-b**

II- NMR Characterizations

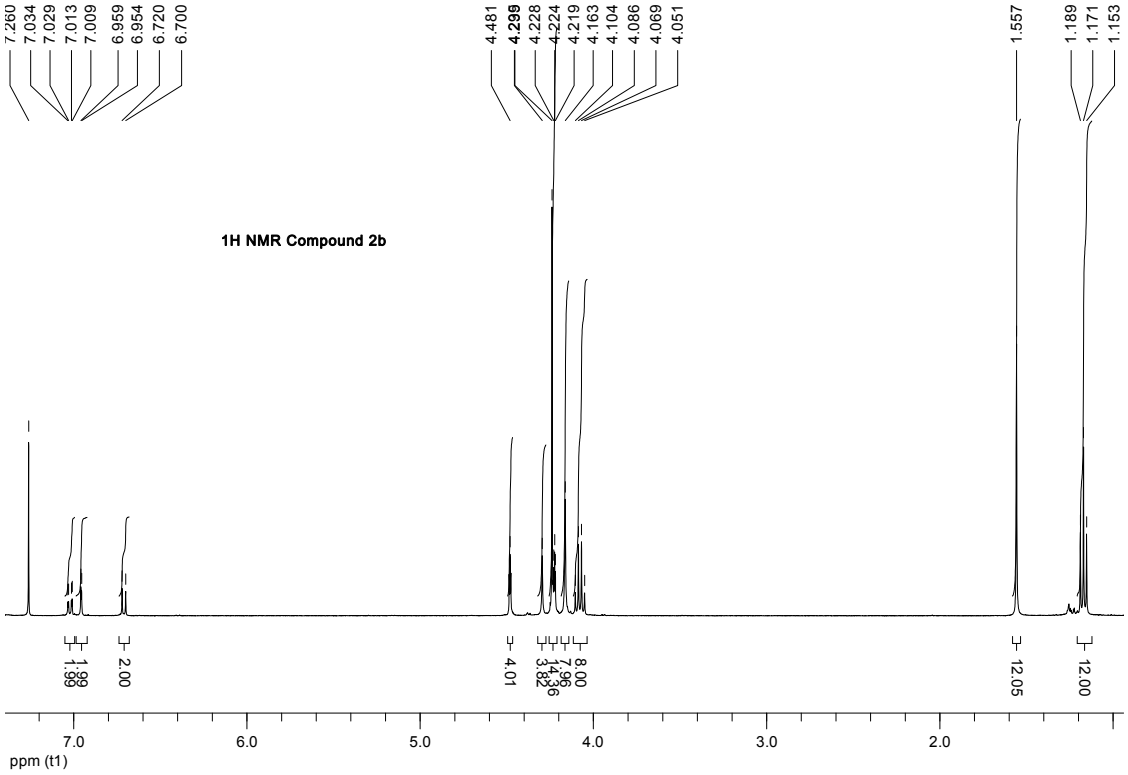


Figure S1: ^{1}H NMR spectrum ($CDCl_3$) of compound **2b**

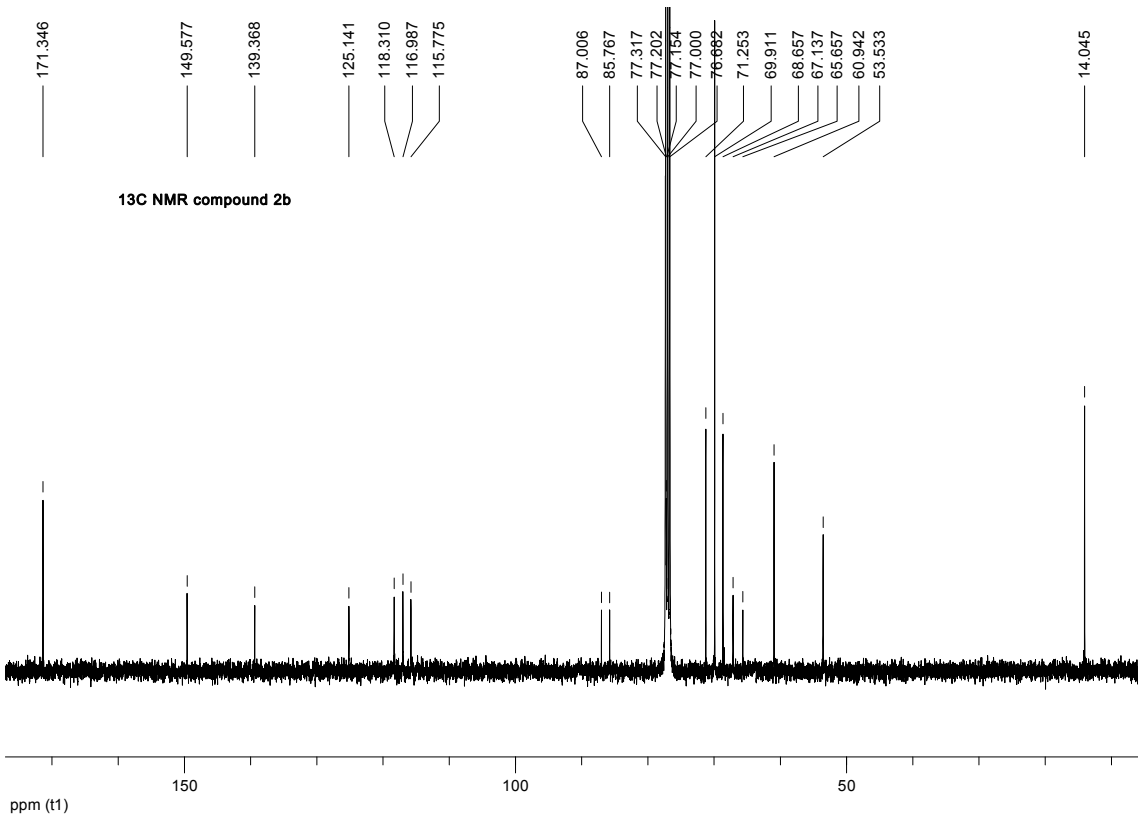


Figure S2: ^{13}C NMR spectrum ($CDCl_3$) of compound **2b**

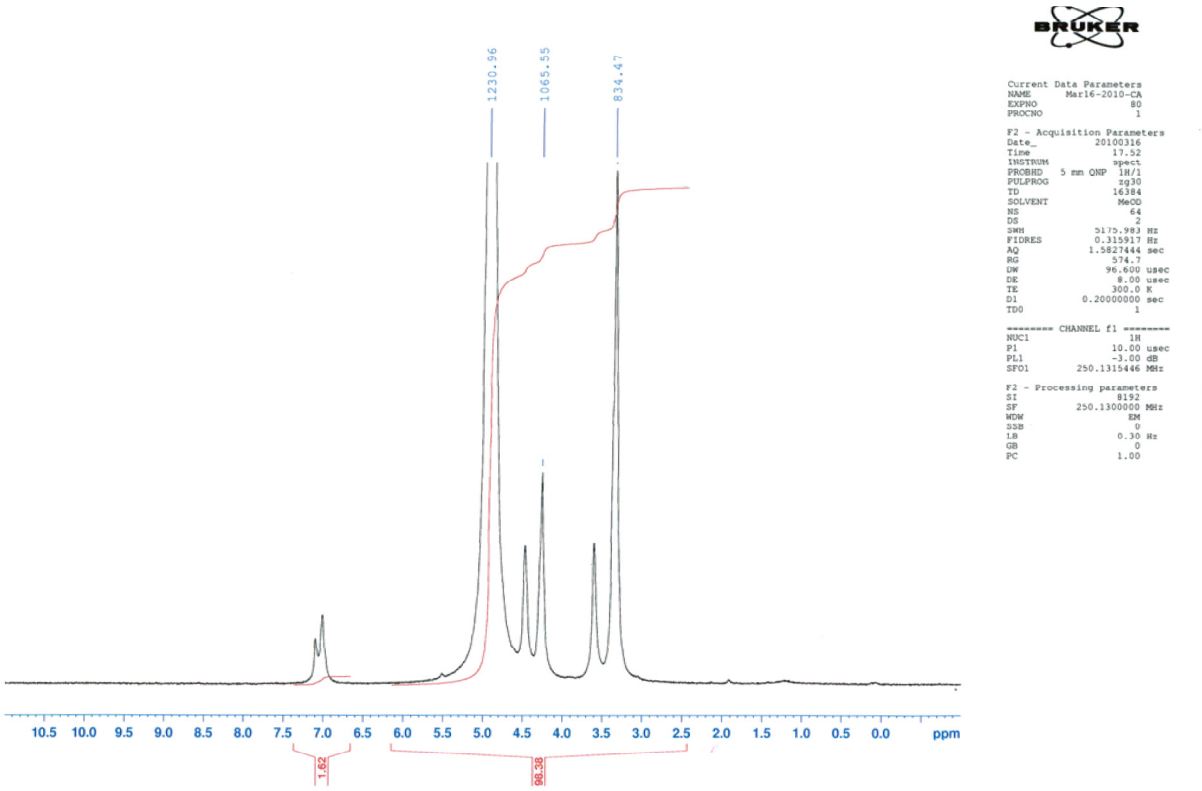


Figure S3: ^{1}H NMR spectrum (CD_3OD) of compound **3b**

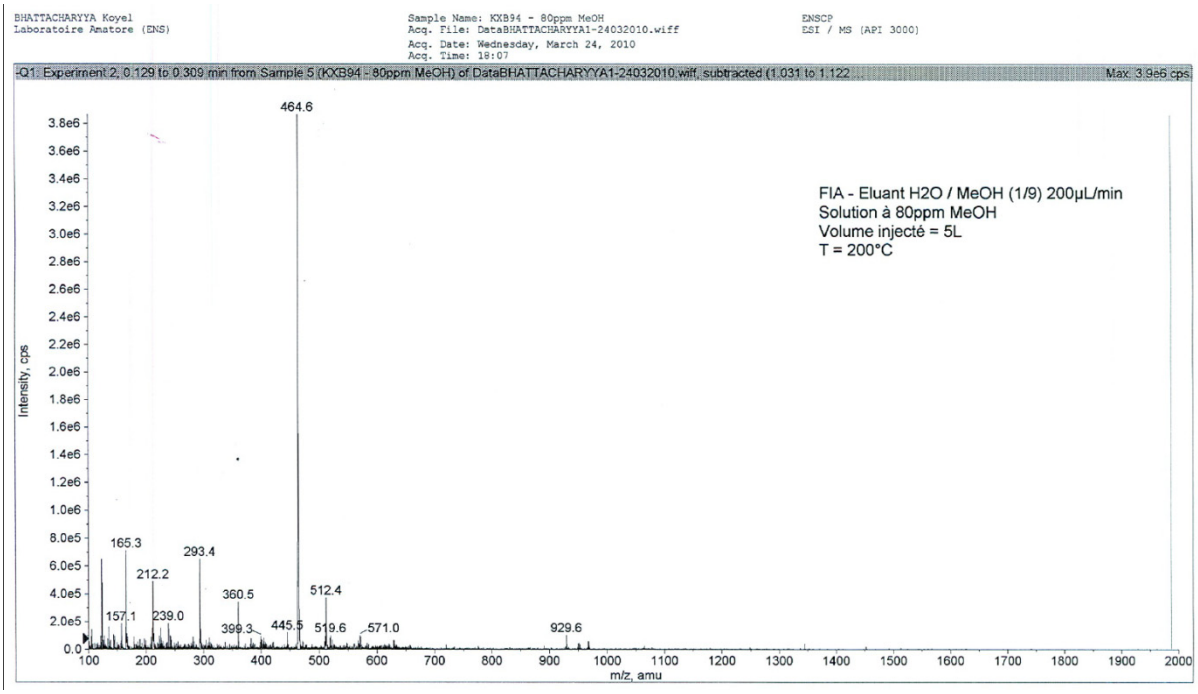


Figure S4: Mass spectrometry characterization by ESI-MS for compound **3b**

III-Electrochemistry

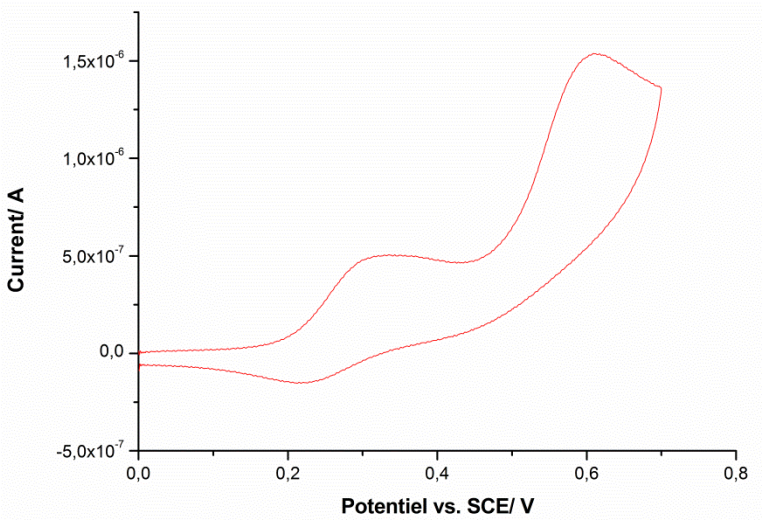


Figure S5: Cyclic Voltammogram of **3b** (1mM) in aqueous electrolyte (0.1 M KCl, 30 mM MOPS, 10 mM EGTA) on glassy carbon electrode (diameter = 1 mm) at 0.1V/s

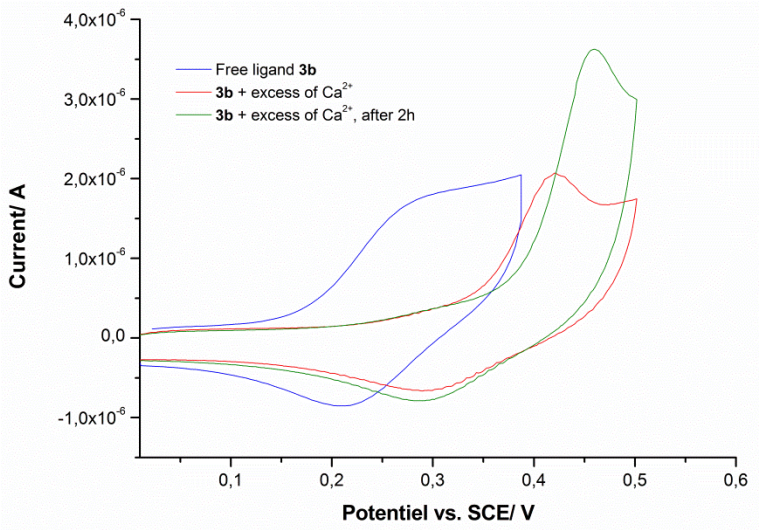


Figure S6: Evolution of the electrochemical response for **3b** in the presence of calcium: **3b** (1 mM) in aqueous electrolyte (0.1 M KCl, 30 mM MOPS, 10 mM EGTA) on glassy carbon electrode (diameter = 1 mm) at 0.5V/s: in the absence of Ca^{2+} (blue line); **3b**+excess of Ca^{2+} (red line); **3b**+excess of Ca^{2+}, after 2h (green line).

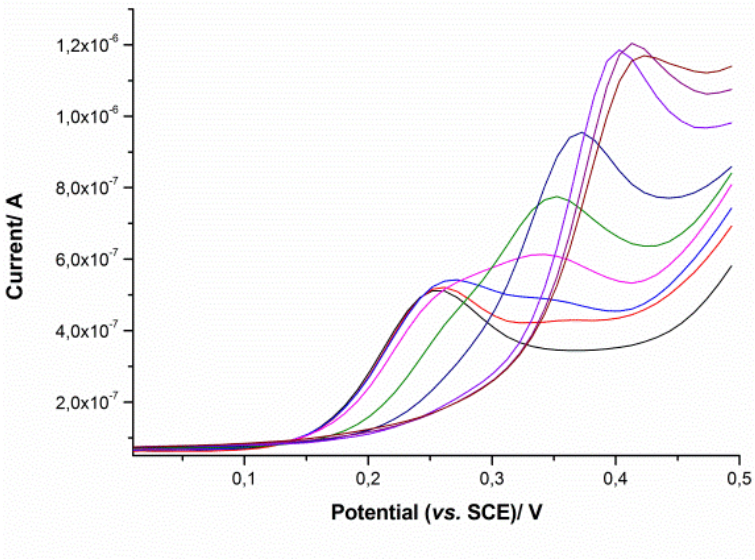
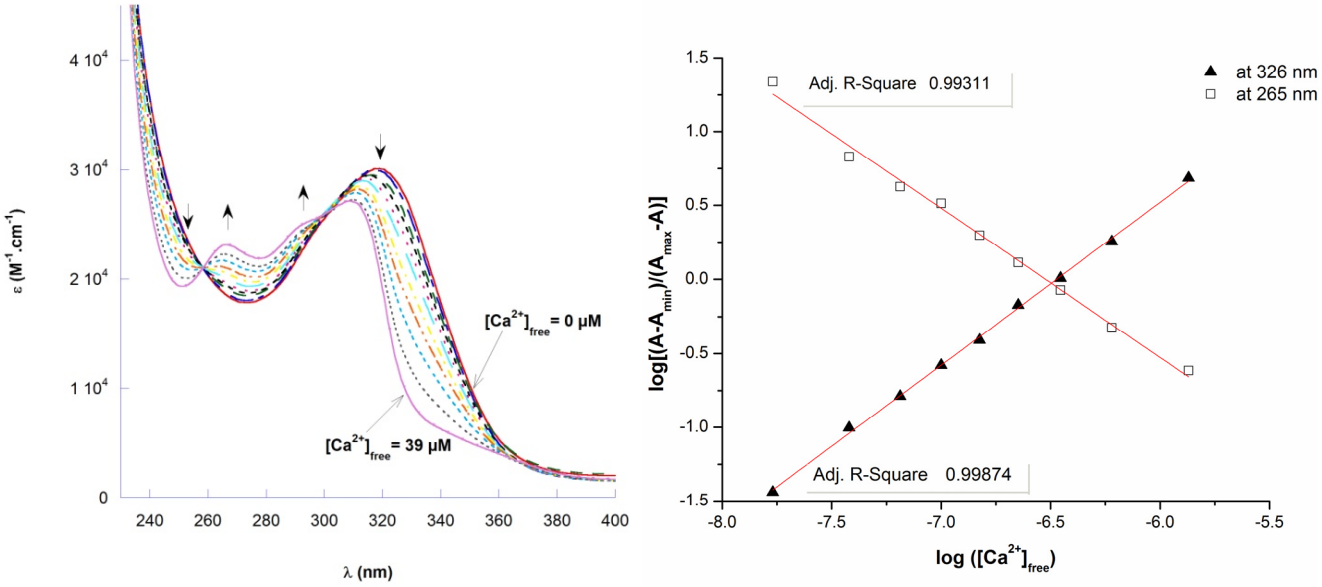


Figure S7: Square wave voltammetry for **3b** on glassy carbon electrode in aqueous solutions (0.1 M KCl, 30 mM MOPS pH=7,4, 10 mM EGTA).

IV- UV-Vis studies

The affinity constant of chelator **3a** for Ca^{2+} was obtained by titration in pH and buffered Ca^{2+} (with 10 mM EGTA as calcium buffer [1,3]) aqueous media and data processed in Hill plot. The latter represents $\log[(A-A_{min})/(A_{max}-A)]$ vs. $\log[Ca^{2+}]_{free}$ at two different wavelengths (266 and 326 nm). A_{min} is the absorbance of the free ligand **3** ($[Ca^{2+}]_{free}= 0$), A_{max} the absorbance of the Ca^{2+} complex ($[Ca^{2+}]_{free}= 39\mu M$), and A the absorbance at a given free Ca^{2+} concentration.



(a) **(b)**

Figure S8: (a) UV-Vis absorption spectra of **3a** for different free Ca^{2+} concentrations set by EGTA buffer (0.1 M KCl, 30mM MOPS pH=7,2, 10mM EGTA). **(b)** Hill plot for absorbance at 265 and 326 nm. A_{min} (A_{max}) is the absorbance of the free ligand **3a** (Ca^{2+} complex, respectively).

The linear behavior with an absolute value of the slope equal 1 is fully consistent with the expected 1:1 complex of calcium (see Figure S8(b)). Furthermore, identical x-axis intercepts for the two selected wavelengths allow us to estimate a dissociation constant K_d^{Ca} of 320±8 nM (at 22±2°C, pH=7.2) for ligand **3a**.

V- Crystallographic data

Figure S9: Molecular structure for **2a**

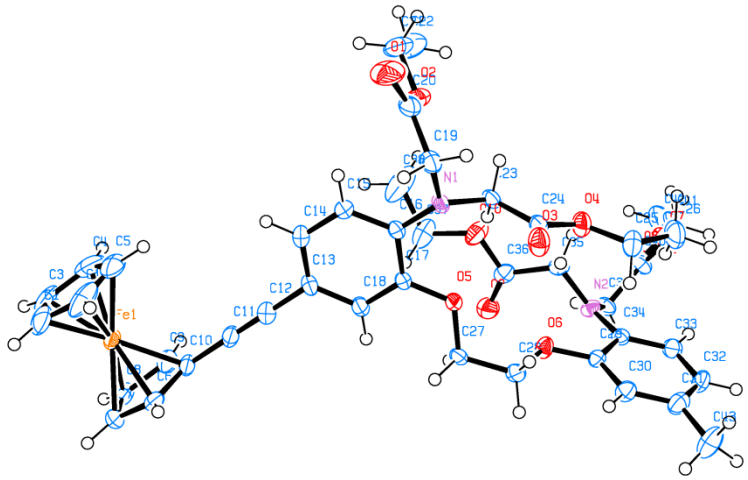


Table S1- 1. Crystal data for **2a.**

Identification code	clb15	
Empirical formula	$C_{43}H_{50}FeN_2O_{10}$, H_2Cl_2	
Formula weight	895.63	
Temperature	200(1) K	
Wavelength	0.71073 Å	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.9797(10) Å	a= 96.115(5)°.
	b = 13.0797(10) Å	b= 101.424(4)°.
	c = 13.7456(11) Å	g = 93.178(4)°.
Volume	2267.3(3) $Å^3$	
Z	2	
Density (calculated)	1.312 Mg/m^3	
Absorption coefficient	0.507 mm^{-1}	
F(000)	940	
Crystal size	0.26 x 0.24 x 0.05 mm^3	
Theta range for data collection	1.97 to 31.74°.	
Index ranges	-19<=h<=18, -19<=k<=19, -19<=l<=20	
Reflections collected	15326	
Independent reflections	9669 [R(int) = 0.0673]	
Completeness to theta = 31.74°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9807 and 0.8803	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9669 / 0 / 537	
Goodness-of-fit on F^2	1.147	
Final R indices [I>2sigma(I)]	R1 = 0.0456, wR2 = 0.0995	
R indices (all data)	R1 = 0.0844, wR2 = 0.1246	
Largest diff. peak and hole	0.841 and -0.922 $e.Å^{-3}$	

Table S1- 2. Atomic coordinates and equivalent isotropic displacement parameters ($Å^2$) for **2a**

Atom	x	y	z	U(eq) [Ang^2]
Fe1	0.54817(4)	-0.21382(3)	0.57538(4)	0.0265(1)
O1	-0.1536(2)	0.1637(3)	0.5469(2)	0.0581(10)
O2	-0.0820(2)	0.1636(2)	0.7089(2)	0.0387(8)
O3	0.0854(2)	0.5178(2)	0.7199(2)	0.0385(9)
O4	0.0774(2)	0.52105(19)	0.88163(18)	0.0329(7)
O5	0.28468(16)	0.36507(17)	0.79840(18)	0.0266(6)
O6	0.35853(19)	0.51689(17)	0.96685(17)	0.0273(7)
O7	0.1701(2)	0.5589(3)	1.2770(2)	0.0465(10)
O8	0.2666(2)	0.4791(2)	1.39550(19)	0.0364(8)
O9	0.3823(2)	0.3126(2)	1.0967(2)	0.0376(8)
O10	0.2191(2)	0.2597(2)	1.0112(2)	0.0421(8)
N1	0.0839(2)	0.3016(2)	0.69940(19)	0.0236(7)
N2	0.3171(2)	0.5075(2)	1.15051(19)	0.0242(7)
C1	0.4413(4)	-0.2313(3)	0.4441(4)	0.0586(16)
C2	0.5144(4)	-0.3061(3)	0.4430(3)	0.0500(14)
C3	0.5094(3)	-0.3649(3)	0.5220(4)	0.0483(13)
C4	0.4325(4)	-0.3259(4)	0.5721(4)	0.0564(16)
C5	0.3905(3)	-0.2432(4)	0.5221(5)	0.0624(16)
C6	0.6262(3)	-0.0730(2)	0.5849(3)	0.0287(9)
C7	0.6994(3)	-0.1499(3)	0.5944(3)	0.0342(10)
C8	0.6874(3)	-0.2007(3)	0.6774(3)	0.0355(10)
C9	0.6070(3)	-0.1569(3)	0.7210(3)	0.0326(10)
C10	0.5684(3)	-0.0761(2)	0.6631(2)	0.0257(8)
C11	0.4841(3)	-0.0143(2)	0.6778(3)	0.0292(9)
C12	0.4140(3)	0.0392(3)	0.6856(3)	0.0316(10)
C13	0.3289(3)	0.1044(3)	0.6901(3)	0.0274(9)
C14	0.2276(3)	0.0739(3)	0.6356(3)	0.0328(10)
C15	0.1473(3)	0.1390(3)	0.6401(3)	0.0292(9)
C16	0.1641(2)	0.2352(2)	0.6977(2)	0.0223(8)
C17	0.2685(2)	0.2667(2)	0.7493(2)	0.0217(8)
C18	0.3486(2)	0.2013(3)	0.7469(3)	0.0264(9)
C19	-0.0076(3)	0.2861(3)	0.6202(3)	0.0305(9)
C20	-0.0889(3)	0.1979(3)	0.6204(3)	0.0341(10)
C21	-0.1587(3)	0.0787(4)	0.7115(4)	0.0532(16)
C22	-0.1383(4)	0.0469(4)	0.8132(4)	0.0682(19)
C23	0.0700(2)	0.3582(2)	0.7922(2)	0.0240(8)
C24	0.0800(2)	0.4738(3)	0.7912(2)	0.0261(8)
C25	0.0771(3)	0.6327(3)	0.8900(3)	0.0404(11)
C26	0.0627(3)	0.6695(3)	0.9935(3)	0.0489(12)

C27	0.3917(2)	0.4062(3)	0.8324(3)	0.0260(8)
C28	0.3911(3)	0.5170(3)	0.8738(2)	0.0260(9)
C29	0.3573(2)	0.6098(2)	1.0227(2)	0.0217(8)
C30	0.3811(3)	0.7047(3)	0.9921(3)	0.0281(9)
C31	0.3841(3)	0.7961(3)	1.0546(3)	0.0337(10)
C32	0.3619(3)	0.7908(3)	1.1483(3)	0.0334(10)
C33	0.3357(3)	0.6968(3)	1.1788(3)	0.0293(9)
C34	0.3337(2)	0.6045(2)	1.1178(2)	0.0222(8)
C35	0.2428(2)	0.4288(3)	1.0892(2)	0.0255(8)
C36	0.2924(3)	0.3293(3)	1.0676(2)	0.0269(9)
C37	0.2544(4)	0.1582(3)	0.9873(3)	0.0497(13)
C38	0.1604(5)	0.0905(4)	0.9311(5)	0.077(2)
C39	0.3387(2)	0.4978(3)	1.2556(2)	0.0257(8)
C40	0.2475(3)	0.5165(3)	1.3086(2)	0.0271(9)
C41	0.1906(3)	0.4949(3)	1.4604(3)	0.0427(12)
C42	0.2233(5)	0.4345(4)	1.5453(4)	0.0626(19)
C43	0.4153(4)	0.8980(3)	1.0213(4)	0.0563(15)

Cl1	0.7694(2)	0.18112(19)	0.24016(16)	0.1296(10)
Cl2	0.9931(3)	0.1855(3)	0.3251(2)	0.1490(14)
C44	0.8758(5)	0.2394(5)	0.3316(4)	0.074(2)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S1- 3. Bond lengths [Å] and angles [°] for **2a.**

Fe1	-C1	2.029(5)	N1	-C19	1.432(5)
Fe1	-C2	2.029(4)	N1	-C23	1.454(4)
Fe1	-C3	2.033(4)	N1	-C16	1.394(4)
Fe1	-C4	2.030(5)	N2	-C39	1.437(4)
Fe1	-C5	2.033(5)	N2	-C34	1.410(4)
Fe1	-C6	2.031(3)	N2	-C35	1.443(4)
Fe1	-C7	2.047(4)	C1	-C5	1.383(8)
Fe1	-C8	2.043(4)	C1	-C2	1.401(7)
Fe1	-C9	2.039(4)	C2	-C3	1.405(6)
Fe1	-C10	2.032(3)	C3	-C4	1.409(7)
Cl1	-C44	1.749(6)	C4	-C5	1.420(8)
Cl2	-C44	1.727(8)	C6	-C10	1.430(5)
O1	-C20	1.205(5)	C6	-C7	1.420(5)
O2	-C21	1.458(5)	C7	-C8	1.410(6)
O2	-C20	1.329(5)	C8	-C9	1.420(6)
O3	-C24	1.200(4)	C9	-C10	1.443(5)
O4	-C25	1.453(5)	C10	-C11	1.429(5)
O4	-C24	1.336(4)	C11	-C12	1.193(5)
O5	-C27	1.430(4)	C12	-C13	1.439(6)
O5	-C17	1.373(3)	C13	-C18	1.398(6)
O6	-C29	1.369(3)	C13	-C14	1.392(6)
O6	-C28	1.425(4)	C14	-C15	1.389(6)
O7	-C40	1.202(5)	C15	-C16	1.395(5)
O8	-C41	1.464(5)	C16	-C17	1.416(4)
O8	-C40	1.322(4)	C17	-C18	1.386(4)
O9	-C36	1.196(5)	C19	-C20	1.520(6)
O10	-C36	1.340(4)	C21	-C22	1.479(8)
O10	-C37	1.454(5)	C23	-C24	1.512(5)
C25	-C26	1.503(6)	C27	-C28	1.501(5)
C29	-C30	1.390(5)	C29	-C34	1.408(4)
C30	-C31	1.390(6)	C31	-C43	1.514(6)
C31	-C32	1.382(6)	C32	-C33	1.387(6)
C33	-C34	1.391(5)	C35	-C36	1.511(5)
C37	-C38	1.494(8)	C39	-C40	1.526(5)
C41	-C42	1.484(7)			

C1	-Fe1	-C2	40.39(19)	C4	-Fe1	-C9	108.10(19)
C1	-Fe1	-C3	68.13(18)	C4	-Fe1	-C10	124.91(18)
C1	-Fe1	-C4	68.1(2)	C5	-Fe1	-C6	123.81(19)
C1	-Fe1	-C5	39.8(2)	C5	-Fe1	-C7	160.7(2)
C1	-Fe1	-C6	106.24(16)	C5	-Fe1	-C8	157.4(2)
C1	-Fe1	-C7	124.56(18)	C5	-Fe1	-C9	121.3(2)

C1	-Fe1	-C8	162.00(19)	C5	-Fe1	-C10	106.69(19)
C1	-Fe1	-C9	155.31(18)	C6	-Fe1	-C7	40.76(15)
C1	-Fe1	-C10	119.17(15)	C6	-Fe1	-C8	68.36(16)
C2	-Fe1	-C3	40.49(19)	C6	-Fe1	-C9	69.32(16)
C2	-Fe1	-C4	68.1(2)	C6	-Fe1	-C10	41.22(15)
C2	-Fe1	-C5	67.5(2)	C7	-Fe1	-C8	40.34(16)
C2	-Fe1	-C6	119.71(17)	C7	-Fe1	-C9	68.77(16)
C2	-Fe1	-C7	107.77(19)	C7	-Fe1	-C10	69.02(16)
C2	-Fe1	-C8	126.05(18)	C8	-Fe1	-C9	40.73(16)
C2	-Fe1	-C9	162.95(17)	C8	-Fe1	-C10	68.87(15)
C2	-Fe1	-C10	154.43(14)	C9	-Fe1	-C10	41.51(14)
C3	-Fe1	-C4	40.58(19)	C20	-O2	-C21	115.0(3)
C3	-Fe1	-C5	68.16(19)	C24	-O4	-C25	116.0(3)
C3	-Fe1	-C6	155.34(17)	C17	-O5	-C27	116.9(2)
C3	-Fe1	-C7	121.31(16)	C28	-O6	-C29	118.1(3)
C3	-Fe1	-C8	109.18(17)	C40	-O8	-C41	117.7(3)
C3	-Fe1	-C9	125.89(18)	C36	-O10	-C37	115.8(3)
C3	-Fe1	-C10	162.80(17)	C16	-N1	-C19	118.8(3)
C4	-Fe1	-C5	40.9(2)	C16	-N1	-C23	121.4(2)
C4	-Fe1	-C6	161.69(19)	C19	-N1	-C23	115.7(3)
C4	-Fe1	-C7	156.69(19)	C34	-N2	-C35	120.7(2)
C4	-Fe1	-C8	122.27(19)	C34	-N2	-C39	119.8(3)
C35	-N2	-C39	115.1(3)	Fe1	-C10	-C6	69.37(16)
Fe1	-C1	-C2	69.8(3)	Fe1	-C10	-C9	69.53(19)
Fe1	-C1	-C5	70.2(3)	Fe1	-C10	-C11	123.9(3)
C2	-C1	-C5	108.3(4)	C6	-C10	-C9	107.4(3)
Fe1	-C2	-C1	69.8(3)	C6	-C10	-C11	126.2(3)
Fe1	-C2	-C3	69.9(2)	C9	-C10	-C11	126.3(3)
C1	-C2	-C3	108.3(4)	C10	-C11	-C12	176.7(4)
Fe1	-C3	-C2	69.6(2)	C11	-C12	-C13	177.3(4)
Fe1	-C3	-C4	69.6(3)	C12	-C13	-C14	120.8(4)
C2	-C3	-C4	107.7(4)	C12	-C13	-C18	119.8(3)
Fe1	-C4	-C3	69.8(3)	C14	-C13	-C18	119.3(3)
Fe1	-C4	-C5	69.7(3)	C13	-C14	-C15	119.6(4)
C3	-C4	-C5	107.3(4)	C14	-C15	-C16	122.3(3)
Fe1	-C5	-C1	70.0(3)	N1	-C16	-C15	122.1(3)
Fe1	-C5	-C4	69.5(3)	N1	-C16	-C17	120.6(2)
C1	-C5	-C4	108.4(4)	C15	-C16	-C17	117.2(3)
Fe1	-C6	-C7	70.21(19)	O5	-C17	-C16	116.1(2)
Fe1	-C6	-C10	69.41(17)	O5	-C17	-C18	123.2(3)
C7	-C6	-C10	108.3(3)	C16	-C17	-C18	120.7(3)
Fe1	-C7	-C6	69.0(2)	C13	-C18	-C17	120.7(3)
Fe1	-C7	-C8	69.7(2)	N1	-C19	-C20	118.4(3)
C6	-C7	-C8	107.9(3)	O1	-C20	-O2	123.9(4)
Fe1	-C8	-C7	70.0(2)	O1	-C20	-C19	122.5(4)
Fe1	-C8	-C9	69.5(2)	O2	-C20	-C19	113.6(3)

C7	-C8	-C9	109.2(3)	O2	-C21	-C22	108.5(4)
Fe1	-C9	-C8	69.8(2)	N1	-C23	-C24	112.8(2)
Fe1	-C9	-C10	68.96(19)	O3	-C24	-O4	124.3(4)
C8	-C9	-C10	107.2(3)	O3	-C24	-C23	126.0(3)
O4	-C24	-C23	109.7(3)	O4	-C25	-C26	107.6(3)
O5	-C27	-C28	108.0(3)	O6	-C28	-C27	106.7(3)
O6	-C29	-C30	124.0(3)	O6	-C29	-C34	115.6(2)
C30	-C29	-C34	120.4(3)	C29	-C30	-C31	121.2(3)
C30	-C31	-C32	118.4(4)	C30	-C31	-C43	120.2(4)
C32	-C31	-C43	121.4(4)	C31	-C32	-C33	120.9(4)
C32	-C33	-C34	121.5(3)	N2	-C34	-C29	119.7(2)
N2	-C34	-C33	122.6(3)	C29	-C34	-C33	117.6(3)
N2	-C35	-C36	112.6(2)	O9	-C36	-O10	124.1(4)
O9	-C36	-C35	126.5(3)	O10	-C36	-C35	109.4(3)
O10	-C37	-C38	107.5(4)	N2	-C39	-C40	115.6(2)
O7	-C40	-O8	124.8(3)	O7	-C40	-C39	125.7(3)
O8	-C40	-C39	109.5(3)	O8	-C41	-C42	106.4(4)

Table S1- 4. Anisotropic displacement parameters for **2a**.

The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$ for **2a**.

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Fe1	0.0255(2)	0.0193(2)	0.0315(3)	-0.0040(2)	0.0015(2)	0.0030(2)
O1	0.0350(15)	0.084(2)	0.0434(17)	-0.0073(16)	-0.0081(12)	-0.0106(15)
O2	0.0287(12)	0.0427(14)	0.0401(15)	-0.0044(12)	0.0045(10)	-0.0097(11)
O3	0.0555(17)	0.0315(13)	0.0337(14)	0.0031(11)	0.0210(12)	0.0067(12)
O4	0.0407(14)	0.0311(12)	0.0273(12)	-0.0036(10)	0.0110(10)	0.0050(10)
O5	0.0176(10)	0.0252(10)	0.0342(12)	-0.0077(9)	0.0045(9)	0.0020(8)
O6	0.0398(13)	0.0217(10)	0.0220(11)	-0.0012(8)	0.0136(9)	-0.0016(9)
O7	0.0337(14)	0.071(2)	0.0440(16)	0.0216(14)	0.0171(12)	0.0234(14)
O8	0.0364(13)	0.0526(16)	0.0306(13)	0.0161(12)	0.0217(11)	0.0181(12)
O9	0.0330(13)	0.0337(13)	0.0458(15)	0.0048(11)	0.0072(11)	0.0026(10)
O10	0.0432(15)	0.0281(12)	0.0478(16)	-0.0018(11)	-0.0028(12)	-0.0047(11)
N1	0.0203(11)	0.0290(13)	0.0208(12)	-0.0034(10)	0.0057(9)	0.0041(10)
N2	0.0261(12)	0.0263(12)	0.0191(12)	0.0018(10)	0.0051(10)	-0.0062(10)
C1	0.070(3)	0.033(2)	0.051(3)	-0.0034(18)	-0.035(2)	0.002(2)
C2	0.062(3)	0.042(2)	0.037(2)	-0.0180(18)	0.0035(19)	-0.0052(19)
C3	0.046(2)	0.0180(15)	0.066(3)	-0.0101(16)	-0.016(2)	0.0007(14)
C4	0.054(3)	0.048(2)	0.060(3)	-0.001(2)	0.007(2)	-0.028(2)
C5	0.0245(18)	0.047(2)	0.098(4)	-0.027(3)	-0.011(2)	0.0040(17)
C6	0.0286(15)	0.0213(14)	0.0338(17)	-0.0008(12)	0.0044(13)	-0.0047(12)
C7	0.0224(15)	0.0314(17)	0.047(2)	-0.0080(15)	0.0094(14)	0.0034(13)
C8	0.0269(16)	0.0237(15)	0.048(2)	-0.0035(14)	-0.0090(14)	0.0077(12)
C9	0.0353(17)	0.0291(16)	0.0302(17)	0.0015(13)	-0.0001(14)	0.0046(13)
C10	0.0259(14)	0.0211(13)	0.0263(15)	-0.0054(11)	-0.0003(12)	0.0052(11)
C11	0.0302(16)	0.0224(14)	0.0321(17)	-0.0056(12)	0.0038(13)	0.0025(12)
C12	0.0334(17)	0.0268(15)	0.0343(18)	-0.0016(13)	0.0088(14)	0.0037(13)
C13	0.0279(15)	0.0253(15)	0.0307(16)	-0.0014(12)	0.0117(13)	0.0068(12)
C14	0.0318(17)	0.0262(16)	0.0392(19)	-0.0077(14)	0.0103(14)	0.0042(13)
C15	0.0229(14)	0.0283(15)	0.0337(17)	-0.0061(13)	0.0056(12)	-0.0014(12)
C16	0.0219(13)	0.0249(14)	0.0214(14)	-0.0003(11)	0.0088(11)	0.0024(11)
C17	0.0205(13)	0.0232(13)	0.0217(14)	-0.0017(11)	0.0076(11)	0.0017(10)
C18	0.0218(14)	0.0279(15)	0.0284(16)	-0.0031(12)	0.0050(12)	0.0046(11)
C19	0.0260(15)	0.0379(18)	0.0256(16)	-0.0011(13)	0.0018(12)	0.0076(13)
C20	0.0210(14)	0.0431(19)	0.0341(18)	-0.0075(15)	0.0020(13)	0.0036(13)
C21	0.038(2)	0.054(3)	0.063(3)	-0.006(2)	0.013(2)	-0.0207(19)
C22	0.059(3)	0.066(3)	0.076(4)	0.016(3)	0.009(3)	-0.022(3)
C23	0.0216(13)	0.0301(15)	0.0222(14)	0.0003(12)	0.0103(11)	0.0035(11)
C24	0.0219(14)	0.0308(15)	0.0259(15)	-0.0016(12)	0.0080(11)	0.0033(12)

C25	0.047(2)	0.0296(17)	0.045(2)	-0.0060(15)	0.0154(17)	0.0044(15)
C26	0.046(2)	0.049(2)	0.046(2)	-0.0188(19)	0.0075(19)	0.0090(19)
C27	0.0188(13)	0.0322(16)	0.0268(15)	-0.0060(12)	0.0101(11)	-0.0013(11)
C28	0.0279(15)	0.0316(16)	0.0192(14)	-0.0022(12)	0.0115(12)	-0.0047(12)
C29	0.0213(13)	0.0213(13)	0.0215(14)	-0.0008(11)	0.0042(10)	-0.0009(10)
C30	0.0320(16)	0.0273(15)	0.0250(15)	0.0036(12)	0.0066(12)	-0.0012(12)
C31	0.0345(17)	0.0245(15)	0.040(2)	0.0047(14)	0.0029(14)	-0.0009(13)
C32	0.0337(17)	0.0246(15)	0.0370(19)	-0.0091(13)	0.0034(14)	-0.0014(13)
C33	0.0269(15)	0.0329(16)	0.0266(16)	-0.0043(13)	0.0070(12)	-0.0013(12)
C34	0.0188(13)	0.0267(14)	0.0197(14)	-0.0012(11)	0.0037(10)	-0.0009(11)
C35	0.0235(14)	0.0291(15)	0.0238(15)	0.0044(12)	0.0053(11)	-0.0028(12)
C36	0.0331(16)	0.0270(15)	0.0217(15)	0.0053(12)	0.0088(12)	-0.0044(12)
C37	0.066(3)	0.0281(18)	0.049(2)	-0.0016(17)	0.002(2)	0.0001(18)
C38	0.103(5)	0.038(2)	0.071(4)	-0.004(2)	-0.018(3)	-0.011(3)
C39	0.0240(14)	0.0341(16)	0.0206(14)	0.0027(12)	0.0086(11)	0.0030(12)
C40	0.0261(15)	0.0336(16)	0.0250(15)	0.0058(13)	0.0116(12)	0.0057(12)
C41	0.044(2)	0.057(2)	0.041(2)	0.0131(18)	0.0340(18)	0.0186(18)
C42	0.083(4)	0.071(3)	0.056(3)	0.030(3)	0.050(3)	0.027(3)
C43	0.078(3)	0.0252(18)	0.063(3)	0.0052(19)	0.011(3)	-0.006(2)

Cl1	0.160(2)	0.1151(16)	0.0886(13)	0.0342(12)	-0.0277(13)	-0.0561(15)
Cl2	0.155(2)	0.176(3)	0.142(2)	0.058(2)	0.0522(19)	0.087(2)
C44	0.099(5)	0.070(4)	0.052(3)	0.020(3)	0.007(3)	-0.002(3)

Table S1- 5. Hydrogen Atom Positions and Isotropic Displacement Parameters for **2a**

Atom	x	y	z	U(iso) [Ang^2]
H1	0.42880	-0.18097	0.39897	0.0702
H2	0.55955	-0.31543	0.39672	0.0600
H3	0.55055	-0.42077	0.53856	0.0578
H4	0.41246	-0.35040	0.62885	0.0672
H5	0.33658	-0.20291	0.53929	0.0745
H6	0.61719	-0.02722	0.53511	0.0345
H7	0.74784	-0.16460	0.55228	0.0410
H8	0.72682	-0.25552	0.70054	0.0425
H9	0.58317	-0.17704	0.77773	0.0391
H14	0.21345	0.00891	0.59563	0.0393
H15	0.07848	0.11727	0.60258	0.0350
H18	0.41762	0.22246	0.78431	0.0317
H19A	-0.04391	0.35071	0.62045	0.0366
H19B	0.01666	0.27568	0.55623	0.0366
H21A	-0.23110	0.10109	0.69476	0.0637
H21B	-0.15224	0.02000	0.66195	0.0637
H22A	-0.13966	0.10665	0.86229	0.1024
H22B	-0.19281	-0.00633	0.81780	0.1024
H22C	-0.06899	0.01914	0.82699	0.1024
H23A	-0.00042	0.33735	0.80428	0.0288
H23B	0.12354	0.33959	0.84816	0.0288
H25A	0.14460	0.66348	0.87877	0.0481
H25B	0.01894	0.65316	0.83935	0.0481
H26A	0.12084	0.64912	1.04287	0.0735
H26B	0.06209	0.74484	1.00128	0.0735
H26C	-0.00432	0.63865	1.00364	0.0735
H27A	0.42821	0.36684	0.88490	0.0312
H27B	0.42930	0.40111	0.77630	0.0312
H28A	0.34148	0.55297	0.82721	0.0311
H28B	0.46238	0.55255	0.88376	0.0311
H30	0.39550	0.70708	0.92720	0.0337
H32	0.36455	0.85235	1.19240	0.0401
H33	0.31878	0.69543	1.24279	0.0352
H35A	0.18415	0.41502	1.12356	0.0306
H35B	0.21279	0.45453	1.02519	0.0306
H37A	0.30846	0.16277	0.94597	0.0595
H37B	0.28560	0.12964	1.04941	0.0595
H38A	0.12768	0.12162	0.87194	0.1153
H38B	0.18241	0.02254	0.91027	0.1153
H38C	0.10939	0.08293	0.97426	0.1153
H39A	0.36053	0.42747	1.26469	0.0308

H39B	0.39921	0.54713	1.28874	0.0308
H41A	0.19139	0.56893	1.48486	0.0513
H41B	0.11845	0.47034	1.42352	0.0513
H42A	0.29518	0.45882	1.58035	0.0935
H42B	0.17512	0.44348	1.59166	0.0935
H42C	0.22116	0.36129	1.52003	0.0935
H43A	0.45038	0.94576	1.07978	0.0845
H43B	0.46348	0.88680	0.97531	0.0845
H43C	0.35205	0.92733	0.98730	0.0845
H44A	0.88409	0.31372	0.32412	0.0889
H44B	0.85992	0.23359	0.39841	0.0889

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The Temperature Factor has the Form of Exp(-T) Where

T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

Figure S10: Molecular structure for **2b**

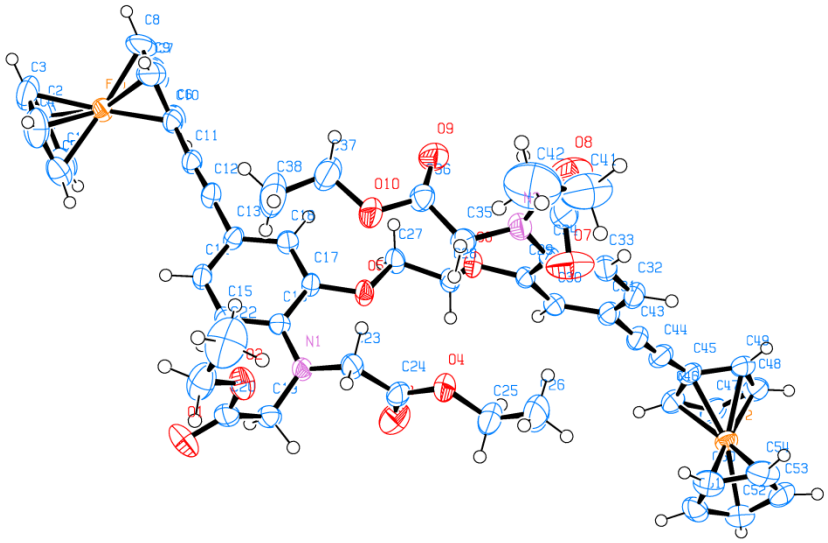

Table S2-1. Crystal data for **2b.**

Identification code	kxb25	
Empirical formula	C54 H56 Fe2 N2 O10	
Formula weight	1004.71	
Temperature	200(1) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.9200(15) Å	a= 69.343(8)°.
	b = 13.1070(14) Å	b= 77.511(7)°
	c = 18.3190(15) Å	g = 62.753(7)°.
Volume	2575.1(5) $Å^3$	
Z	2	
Density (calculated)	1.296 Mg/m^3	
Absorption coefficient	0.621 mm^{-1}	
F(000)	1052	
Crystal size	0.27 x 0.25 x 0.20 mm^3	
Theta range for data collection	1.78 to 30.00°.	
Index ranges	-18<=h<=18, -18<=k<=18, -25<=l<=25	
Reflections collected	14955	
Independent reflections	6751 [R(int) = 0.0446]	
Completeness to theta = 30°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9027 and 0.8902	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14955 / 0 / 617	
Goodness-of-fit on F^2	1.018	
Final R indices [I>2sigma(I)]	R1 = 0.0501, wR2 = 0.0851	
R indices (all data)	R1 = 0.1139, wR2 = 0.1084	
Largest diff. peak and hole	0.818 and -0.291 $e.Å^{-3}$	

Table S2- 2. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for **2b.**

Atom	x	y	z	U(eq) [Ang^2]
Fe1	1.11847(4)	0.24865(4)	0.62574(3)	0.0377(2)
Fe2	0.70296(4)	1.11495(4)	-0.40834(3)	0.0349(2)
O1	0.76183(17)	0.5324(2)	0.17488(11)	0.0406(8)
O2	0.3152(2)	0.5357(3)	0.39057(16)	0.0667(11)
O3	0.4248(2)	0.4169(2)	0.31664(13)	0.0467(9)
O4	0.5153(2)	0.7407(3)	0.10400(16)	0.0632(11)
O5	0.5510(2)	0.6108(2)	0.03849(13)	0.0592(10)
O6	0.85300(18)	0.50773(18)	0.02214(11)	0.0361(8)
O7	0.9891(2)	0.2214(2)	0.10095(14)	0.0571(10)
O8	0.8247(2)	0.2402(2)	0.17643(13)	0.0528(9)
O9	0.7310(2)	0.2778(2)	-0.10263(19)	0.0758(13)
O10	0.8701(3)	0.0925(2)	-0.08361(18)	0.0717(11)
N1	0.5445(2)	0.5597(2)	0.24549(14)	0.0330(8)
N2	0.8669(2)	0.3334(2)	-0.03336(15)	0.0390(9)
C1	0.8680(3)	0.5397(3)	0.13741(17)	0.0355(10)
C2	0.7533(3)	0.4931(3)	0.25494(16)	0.0290(10)
C3	0.6404(3)	0.5089(3)	0.28966(17)	0.0288(10)
C4	0.6288(3)	0.4794(3)	0.37057(17)	0.0350(11)
C5	0.7215(3)	0.4332(3)	0.41572(18)	0.0377(11)
C6	0.8318(3)	0.4128(3)	0.38124(17)	0.0321(10)
C7	0.8474(3)	0.4427(3)	0.30029(17)	0.0333(10)
C8	0.9308(3)	0.3627(3)	0.42794(18)	0.0352(11)
C9	1.0090(3)	0.3227(3)	0.46742(18)	0.0359(11)
C10	1.1077(3)	0.2748(3)	0.51060(18)	0.0404(11)
C11	1.1625(3)	0.3424(4)	0.5193(2)	0.0539(14)
C12	1.2619(3)	0.2607(5)	0.5616(2)	0.073(2)
C13	1.2694(3)	0.1468(5)	0.5790(3)	0.0771(18)
C14	1.1746(3)	0.1521(4)	0.5488(2)	0.0603(16)
C15	0.9537(3)	0.3180(4)	0.6746(2)	0.0551(14)
C16	1.0188(4)	0.3721(4)	0.6831(2)	0.0590(17)
C17	1.1154(4)	0.2833(4)	0.7249(2)	0.0646(18)
C18	1.1114(4)	0.1732(4)	0.7421(2)	0.0723(18)
C19	1.0098(4)	0.1951(4)	0.7108(2)	0.070(2)
C20	0.4293(3)	0.6063(3)	0.28168(18)	0.0375(11)
C21	0.3833(3)	0.5160(3)	0.33590(19)	0.0386(11)
C22	0.3800(4)	0.3292(4)	0.3657(2)	0.0596(16)
C23	0.4340(5)	0.2257(4)	0.3349(3)	0.098(2)
C24	0.5517(3)	0.5353(3)	0.17339(17)	0.0365(11)
C25	0.5375(3)	0.6434(4)	0.1032(2)	0.0459(14)
C26	0.5221(4)	0.7071(4)	-0.0326(2)	0.0811(18)

C27	0.5238(4)	0.6557(5)	-0.0942(3)	0.107(2)
C28	0.8520(3)	0.5953(3)	0.05208(17)	0.0346(10)
C29	0.8418(3)	0.5372(3)	-0.05595(17)	0.0316(10)
C30	0.8490(3)	0.4473(3)	-0.08379(17)	0.0328(10)
C31	0.8453(3)	0.4732(3)	-0.16366(18)	0.0393(11)
C32	0.8359(3)	0.5836(3)	-0.21449(19)	0.0434(11)
C33	0.8278(3)	0.6724(3)	-0.18703(18)	0.0397(11)
C34	0.8305(3)	0.6490(3)	-0.10644(18)	0.0359(11)
C35	0.8224(3)	0.7856(3)	-0.23945(19)	0.0455(11)
C36	0.8226(3)	0.8764(3)	-0.2832(2)	0.0442(12)
C37	0.8294(3)	0.9821(3)	-0.33833(19)	0.0411(11)
C38	0.7975(3)	1.0941(3)	-0.3257(2)	0.0468(12)
C39	0.8184(3)	1.1729(3)	-0.3961(2)	0.0461(12)
C40	0.8630(3)	1.1109(3)	-0.4519(2)	0.0471(12)
C41	0.8704(3)	0.9940(3)	-0.41783(19)	0.0415(11)
C42	0.5616(3)	1.0758(3)	-0.3775(2)	0.0506(14)
C43	0.5320(3)	1.1895(3)	-0.3720(2)	0.0494(14)
C44	0.5544(3)	1.2606(3)	-0.4460(2)	0.0508(14)
C45	0.5976(3)	1.1909(4)	-0.4980(2)	0.0568(14)
C46	0.6021(3)	1.0751(4)	-0.4548(3)	0.0575(16)
C47	0.8050(3)	0.3175(3)	0.04236(18)	0.0383(11)
C48	0.8860(3)	0.2548(3)	0.10834(19)	0.0420(12)
C49	0.8922(4)	0.1771(4)	0.2451(2)	0.0651(16)
C50	0.8106(5)	0.1627(4)	0.3145(2)	0.090(2)
C51	0.9152(3)	0.2316(3)	-0.0622(2)	0.0449(12)
C52	0.8269(3)	0.2061(3)	-0.0856(2)	0.0472(12)
C53	0.7927(5)	0.0516(4)	-0.1025(3)	0.093(2)
C54	0.7528(5)	-0.0199(5)	-0.0316(4)	0.120(3)

U(eq) = 1/3 of the trace of the orthogonalized U Tensor

Table S2- 3. Bond lengths [Å] and angles [°] for **2b.**

Fe1	-C10	2.039(3)	O6	-C28	1.430(4)
Fe1	-C11	2.026(4)	O6	-C29	1.366(4)
Fe1	-C12	2.009(5)	O7	-C48	1.189(5)
Fe1	-C13	2.005(6)	O8	-C48	1.328(4)
Fe1	-C14	2.022(4)	O8	-C49	1.452(5)
Fe1	-C15	2.034(5)	O9	-C52	1.187(5)
Fe1	-C16	2.022(5)	O10	-C52	1.319(4)
Fe1	-C17	2.011(4)	O10	-C53	1.476(8)
Fe1	-C18	2.010(3)	N1	-C3	1.390(5)
Fe1	-C19	2.019(5)	N1	-C20	1.433(5)
Fe2	-C37	2.018(4)	N1	-C24	1.440(4)
Fe2	-C38	2.015(4)	N2	-C30	1.392(4)
Fe2	-C39	2.038(4)	N2	-C47	1.441(4)
Fe2	-C40	2.032(4)	N2	-C51	1.429(4)
Fe2	-C41	2.029(4)	C1	-C28	1.488(4)
Fe2	-C42	2.031(4)	C2	-C3	1.411(6)
Fe2	-C43	2.031(4)	C2	-C7	1.385(5)
Fe2	-C44	2.023(4)	C3	-C4	1.386(4)
Fe2	-C45	2.028(4)	C4	-C5	1.377(6)
Fe2	-C46	2.028(5)	C5	-C6	1.372(6)
O1	-C1	1.424(5)	C6	-C7	1.388(4)
O1	-C2	1.370(3)	C6	-C8	1.452(6)
O2	-C21	1.199(5)	C8	-C9	1.176(6)
O3	-C21	1.305(4)	C9	-C10	1.414(6)
O3	-C22	1.456(5)	C10	-C11	1.426(6)
O4	-C25	1.177(6)	C10	-C14	1.421(6)
O5	-C25	1.348(5)	C11	-C12	1.408(7)
O5	-C26	1.431(4)	C12	-C13	1.373(8)
C13	-C14	1.414(7)	C45	-C46	1.423(7)
C15	-C16	1.384(7)	C47	-C48	1.513(5)
C15	-C19	1.395(6)	C49	-C50	1.482(7)
C16	-C17	1.398(7)	C51	-C52	1.503(6)
C17	-C18	1.387(7)	C53	-C54	1.458(9)
C18	-C19	1.414(8)	C20	-C21	1.517(5)
C22	-C23	1.466(7)	C24	-C25	1.508(5)
C26	-C27	1.497(7)	C29	-C30	1.400(5)
C29	-C34	1.389(5)	C30	-C31	1.387(4)
C31	-C32	1.383(5)	C32	-C33	1.378(5)
C33	-C34	1.403(4)	C33	-C35	1.434(5)
C35	-C36	1.178(5)	C36	-C37	1.426(5)
C37	-C38	1.422(5)	C37	-C41	1.417(5)
C38	-C39	1.403(5)	C39	-C40	1.393(5)
C40	-C41	1.401(5)	C42	-C43	1.395(5)
C42	-C46	1.401(6)	C43	-C44	1.406(5)

C44	-C45	1.404(6)					
C10	-Fe1	-C11	41.08(17)	C13	-Fe1	-C18	108.8(2)
C10	-Fe1	-C12	68.73(17)	C13	-Fe1	-C19	128.3(2)
C10	-Fe1	-C13	68.56(19)	C14	-Fe1	-C15	127.13(18)
C10	-Fe1	-C14	40.94(16)	C14	-Fe1	-C16	162.33(19)
C10	-Fe1	-C15	108.21(16)	C14	-Fe1	-C17	156.54(19)
C10	-Fe1	-C16	124.06(16)	C14	-Fe1	-C18	122.63(18)
C10	-Fe1	-C17	160.31(17)	C14	-Fe1	-C19	110.35(18)
C10	-Fe1	-C18	158.05(19)	C15	-Fe1	-C16	39.9(2)
C10	-Fe1	-C19	122.35(18)	C15	-Fe1	-C17	67.8(2)
C11	-Fe1	-C12	40.84(18)	C15	-Fe1	-C18	68.46(19)
C11	-Fe1	-C13	68.2(2)	C15	-Fe1	-C19	40.25(18)
C11	-Fe1	-C14	69.06(18)	C16	-Fe1	-C17	40.56(19)
C11	-Fe1	-C15	119.51(18)	C16	-Fe1	-C18	68.21(17)
C11	-Fe1	-C16	105.31(18)	C16	-Fe1	-C19	67.54(19)
C11	-Fe1	-C17	122.61(19)	C17	-Fe1	-C18	40.37(19)
C11	-Fe1	-C18	160.0(2)	C17	-Fe1	-C19	68.0(2)
C11	-Fe1	-C19	155.76(19)	C18	-Fe1	-C19	41.1(2)
C12	-Fe1	-C13	40.0(2)	C37	-Fe2	-C38	41.30(15)
C12	-Fe1	-C14	68.7(2)	C37	-Fe2	-C39	68.92(16)
C12	-Fe1	-C15	153.7(2)	C37	-Fe2	-C40	68.30(15)
C12	-Fe1	-C16	118.7(2)	C37	-Fe2	-C41	41.00(14)
C12	-Fe1	-C17	105.9(2)	C37	-Fe2	-C42	106.73(16)
C12	-Fe1	-C18	124.2(2)	C37	-Fe2	-C43	124.29(15)
C12	-Fe1	-C19	163.2(2)	C37	-Fe2	-C44	161.68(14)
C13	-Fe1	-C14	41.1(2)	C37	-Fe2	-C45	155.77(17)
C13	-Fe1	-C15	165.2(2)	C37	-Fe2	-C46	119.88(18)
C13	-Fe1	-C16	154.0(2)	C38	-Fe2	-C39	40.49(15)
C13	-Fe1	-C17	120.2(2)	C38	-Fe2	-C40	67.63(15)
C38	-Fe2	-C41	68.66(15)	C43	-Fe2	-C44	40.58(14)
C38	-Fe2	-C42	120.40(15)	C43	-Fe2	-C45	68.25(16)
C38	-Fe2	-C43	107.41(15)	C43	-Fe2	-C46	67.90(18)
C38	-Fe2	-C44	124.81(15)	C44	-Fe2	-C45	40.55(16)
C38	-Fe2	-C45	161.84(17)	C44	-Fe2	-C46	68.36(18)
C38	-Fe2	-C46	155.38(18)	C45	-Fe2	-C46	41.08(19)
C39	-Fe2	-C40	40.02(15)	C1	-O1	-C2	117.8(3)
C39	-Fe2	-C41	68.28(16)	C21	-O3	-C22	115.2(3)
C39	-Fe2	-C42	155.54(14)	C25	-O5	-C26	115.4(3)
C39	-Fe2	-C43	121.15(15)	C28	-O6	-C29	118.6(2)
C39	-Fe2	-C44	108.10(16)	C48	-O8	-C49	115.6(3)
C39	-Fe2	-C45	125.37(16)	C52	-O10	-C53	117.5(4)
C39	-Fe2	-C46	162.80(18)	C3	-N1	-C20	119.4(3)
C40	-Fe2	-C41	40.37(15)	C3	-N1	-C24	122.3(3)
C40	-Fe2	-C42	162.62(15)	C20	-N1	-C24	115.4(3)

C40	-Fe2	-C43	156.34(15)	C30	-N2	-C47	121.3(3)
C40	-Fe2	-C44	121.81(15)	C30	-N2	-C51	120.9(3)
C40	-Fe2	-C45	108.83(16)	C47	-N2	-C51	114.7(3)
C40	-Fe2	-C46	126.36(18)	O1	-C1	-C28	107.7(3)
C41	-Fe2	-C42	125.11(15)	O1	-C2	-C3	115.6(3)
C41	-Fe2	-C43	161.66(15)	O1	-C2	-C7	123.4(3)
C41	-Fe2	-C44	156.27(14)	C3	-C2	-C7	121.0(3)
C41	-Fe2	-C45	121.07(16)	N1	-C3	-C2	122.2(3)
C41	-Fe2	-C46	107.78(18)	N1	-C3	-C4	121.6(4)
C42	-Fe2	-C43	40.16(15)	C2	-C3	-C4	116.1(3)
C42	-Fe2	-C44	68.08(16)	C3	-C4	-C5	122.9(4)
C42	-Fe2	-C45	68.46(16)	C4	-C5	-C6	120.3(3)
C42	-Fe2	-C46	40.39(17)	C5	-C6	-C7	118.8(4)
C5	-C6	-C8	121.1(3)	C15	-C16	-C17	108.4(4)
C7	-C6	-C8	120.1(4)	Fe1	-C17	-C16	70.2(2)
C2	-C7	-C6	120.7(4)	Fe1	-C17	-C18	69.8(2)
C6	-C8	-C9	178.3(4)	C16	-C17	-C18	108.5(5)
C8	-C9	-C10	176.4(4)	Fe1	-C18	-C17	69.8(2)
Fe1	-C10	-C9	130.3(3)	Fe1	-C18	-C19	69.8(2)
Fe1	-C10	-C11	69.0(2)	C17	-C18	-C19	107.0(4)
Fe1	-C10	-C14	68.9(2)	Fe1	-C19	-C15	70.5(3)
C9	-C10	-C11	125.2(3)	Fe1	-C19	-C18	69.1(3)
C9	-C10	-C14	127.2(4)	C15	-C19	-C18	108.2(4)
C11	-C10	-C14	107.4(4)	N1	-C20	-C21	117.2(3)
Fe1	-C11	-C10	70.0(2)	O2	-C21	-O3	124.3(4)
Fe1	-C11	-C12	68.9(2)	O2	-C21	-C20	122.4(3)
C10	-C11	-C12	107.5(4)	O3	-C21	-C20	113.3(3)
Fe1	-C12	-C11	70.3(3)	O3	-C22	-C23	107.6(4)
Fe1	-C12	-C13	69.8(3)	N1	-C24	-C25	112.4(3)
C11	-C12	-C13	108.7(4)	O4	-C25	-O5	125.3(3)
Fe1	-C13	-C12	70.2(3)	O4	-C25	-C24	126.5(3)
Fe1	-C13	-C14	70.1(3)	O5	-C25	-C24	108.2(4)
C12	-C13	-C14	109.4(5)	O5	-C26	-C27	107.1(4)
Fe1	-C14	-C10	70.2(2)	O6	-C28	-C1	107.6(3)
Fe1	-C14	-C13	68.8(3)	O6	-C29	-C30	117.0(3)
C10	-C14	-C13	107.0(4)	O6	-C29	-C34	121.7(3)
Fe1	-C15	-C16	69.6(3)	C30	-C29	-C34	121.3(3)
Fe1	-C15	-C19	69.3(3)	N2	-C30	-C29	120.8(3)
C16	-C15	-C19	107.9(4)	N2	-C30	-C31	121.3(3)
Fe1	-C16	-C15	70.5(3)	C29	-C30	-C31	117.8(3)
Fe1	-C16	-C17	69.3(3)	C30	-C31	-C32	121.4(3)
C31	-C32	-C33	120.8(3)	Fe2	-C43	-C42	69.9(2)
C32	-C33	-C34	119.0(3)	Fe2	-C43	-C44	69.4(2)
C32	-C33	-C35	121.3(3)	C42	-C43	-C44	108.3(3)
C34	-C33	-C35	119.6(3)	Fe2	-C44	-C43	70.0(2)
C29	-C34	-C33	119.7(3)	Fe2	-C44	-C45	69.9(2)

C33	-C35	-C36	177.4(4)	C43	-C44	-C45	108.3(3)
C35	-C36	-C37	176.5(4)	Fe2	-C45	-C44	69.5(2)
Fe2	-C37	-C36	125.8(3)	Fe2	-C45	-C46	69.4(3)
Fe2	-C37	-C38	69.3(2)	C44	-C45	-C46	107.2(3)
Fe2	-C37	-C41	69.9(2)	Fe2	-C46	-C42	69.9(3)
C36	-C37	-C38	127.9(3)	Fe2	-C46	-C45	69.5(3)
C36	-C37	-C41	125.2(3)	C42	-C46	-C45	107.9(4)
C38	-C37	-C41	106.9(3)	N2	-C47	-C48	112.3(3)
Fe2	-C38	-C37	69.5(2)	O7	-C48	-O8	124.7(3)
Fe2	-C38	-C39	70.6(2)	O7	-C48	-C47	125.7(3)
C37	-C38	-C39	108.7(3)	O8	-C48	-C47	109.6(3)
Fe2	-C39	-C38	68.9(2)	O8	-C49	-C50	107.8(4)
Fe2	-C39	-C40	69.8(2)	N2	-C51	-C52	114.7(3)
C38	-C39	-C40	107.4(3)	O9	-C52	-O10	124.6(4)
Fe2	-C40	-C39	70.2(2)	O9	-C52	-C51	124.8(3)
Fe2	-C40	-C41	69.7(2)	O10	-C52	-C51	110.6(4)
C39	-C40	-C41	109.5(3)	O10	-C53	-C54	110.4(5)
Fe2	-C41	-C37	69.1(2)	Fe2	-C41	-C40	70.0(2)
C37	-C41	-C40	107.6(3)	Fe2	-C42	-C43	69.9(2)
Fe2	-C42	-C46	69.7(3)	C43	-C42	-C46	108.3(3)

Table S2- 4. Anisotropic displacement parameters ($Å^2$) for **2b**.

The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

Atom	U(1,1) or U	U(2,2)	U(3,3)	U(2,3)	U(1,3)	U(1,2)
Fe1	0.0354(3)	0.0492(3)	0.0328(3)	-0.0141(2)	-0.0061(2)	-0.0179(2)
Fe2	0.0305(3)	0.0384(3)	0.0356(3)	-0.0074(2)	-0.0063(2)	-0.0149(2)
O1	0.0274(12)	0.0723(16)	0.0230(12)	-0.0082(11)	-0.0003(9)	-0.0263(12)
O2	0.0498(17)	0.084(2)	0.0621(18)	-0.0347(16)	0.0265(14)	-0.0276(16)
O3	0.0557(16)	0.0532(15)	0.0415(14)	-0.0172(12)	0.0062(11)	-0.0328(13)
O4	0.073(2)	0.0547(18)	0.0590(18)	-0.0014(14)	-0.0161(14)	-0.0304(16)
O5	0.0490(16)	0.0836(19)	0.0295(14)	-0.0153(13)	-0.0051(11)	-0.0148(14)
O6	0.0461(14)	0.0402(13)	0.0217(12)	-0.0058(10)	-0.0012(9)	-0.0205(11)
O7	0.0404(16)	0.0671(18)	0.0538(16)	-0.0112(14)	-0.0071(12)	-0.0172(14)
O8	0.0531(16)	0.0593(16)	0.0329(14)	-0.0010(12)	0.0006(11)	-0.0232(13)
O9	0.0497(18)	0.0526(17)	0.126(3)	-0.0307(17)	-0.0313(17)	-0.0077(15)
O10	0.071(2)	0.0452(16)	0.098(2)	-0.0275(15)	-0.0318(16)	-0.0075(15)
N1	0.0270(14)	0.0472(16)	0.0252(14)	-0.0108(12)	-0.0015(10)	-0.0158(13)
N2	0.0435(17)	0.0382(16)	0.0343(16)	-0.0113(13)	0.0027(12)	-0.0181(14)
C1	0.0290(17)	0.057(2)	0.0283(17)	-0.0129(15)	0.0026(13)	-0.0259(16)
C2	0.0317(17)	0.0358(17)	0.0220(16)	-0.0060(13)	-0.0009(12)	-0.0183(15)
C3	0.0286(17)	0.0287(16)	0.0298(17)	-0.0094(13)	-0.0023(13)	-0.0117(14)
C4	0.0310(18)	0.046(2)	0.0275(18)	-0.0112(15)	0.0037(13)	-0.0178(16)
C5	0.0383(19)	0.049(2)	0.0238(17)	-0.0066(15)	-0.0016(14)	-0.0198(17)
C6	0.0331(18)	0.0374(18)	0.0265(17)	-0.0034(14)	-0.0072(13)	-0.0175(15)
C7	0.0319(18)	0.0405(18)	0.0317(18)	-0.0106(14)	-0.0026(13)	-0.0183(15)
C8	0.0398(19)	0.0417(19)	0.0273(17)	-0.0054(14)	-0.0017(14)	-0.0233(16)
C9	0.0357(19)	0.046(2)	0.0271(17)	-0.0100(15)	-0.0031(14)	-0.0180(16)
C10	0.0334(19)	0.057(2)	0.0275(18)	-0.0137(16)	-0.0038(14)	-0.0144(17)
C11	0.042(2)	0.084(3)	0.041(2)	-0.011(2)	0.0021(16)	-0.038(2)
C12	0.038(2)	0.136(5)	0.055(3)	-0.034(3)	0.0015(19)	-0.042(3)
C13	0.038(2)	0.105(4)	0.060(3)	-0.045(3)	-0.020(2)	0.016(3)
C14	0.058(3)	0.062(3)	0.051(2)	-0.032(2)	-0.0191(19)	0.001(2)
C15	0.045(2)	0.077(3)	0.051(2)	-0.028(2)	0.0108(18)	-0.031(2)
C16	0.066(3)	0.067(3)	0.056(3)	-0.035(2)	0.012(2)	-0.032(2)
C17	0.082(3)	0.102(4)	0.040(2)	-0.032(2)	0.005(2)	-0.059(3)
C18	0.083(3)	0.092(4)	0.032(2)	-0.002(2)	-0.011(2)	-0.037(3)
C19	0.091(4)	0.094(4)	0.051(3)	-0.016(2)	0.010(2)	-0.070(3)
C20	0.0307(18)	0.042(2)	0.0379(19)	-0.0150(16)	-0.0053(14)	-0.0099(16)
C21	0.0252(18)	0.052(2)	0.039(2)	-0.0152(17)	-0.0044(15)	-0.0140(17)
C22	0.068(3)	0.075(3)	0.046(2)	0.001(2)	-0.0106(19)	-0.049(2)
C23	0.151(5)	0.075(3)	0.091(4)	-0.020(3)	-0.015(4)	-0.067(4)
C24	0.0333(18)	0.051(2)	0.0320(18)	-0.0163(16)	-0.0029(14)	-0.0198(16)
C25	0.0304(19)	0.069(3)	0.033(2)	-0.0068(19)	-0.0075(15)	-0.020(2)

C26	0.062(3)	0.115(4)	0.034(2)	-0.002(2)	-0.0072(19)	-0.023(3)
C27	0.067(3)	0.187(6)	0.043(3)	-0.033(3)	-0.012(2)	-0.031(4)
C28	0.0344(18)	0.0419(19)	0.0271(17)	-0.0068(14)	0.0026(13)	-0.0201(16)
C29	0.0240(16)	0.0415(19)	0.0245(17)	-0.0065(14)	0.0011(12)	-0.0131(14)
C30	0.0264(17)	0.0424(19)	0.0282(18)	-0.0087(15)	0.0007(13)	-0.0155(15)
C31	0.0352(19)	0.050(2)	0.034(2)	-0.0146(16)	-0.0007(14)	-0.0178(16)
C32	0.040(2)	0.058(2)	0.0270(18)	-0.0061(17)	-0.0066(14)	-0.0189(18)
C33	0.0305(18)	0.051(2)	0.0295(19)	-0.0024(16)	-0.0007(14)	-0.0178(17)
C34	0.0313(18)	0.0408(19)	0.0315(18)	-0.0099(15)	-0.0002(13)	-0.0131(15)
C35	0.038(2)	0.056(2)	0.0288(19)	-0.0023(18)	-0.0038(14)	-0.0151(18)
C36	0.038(2)	0.049(2)	0.037(2)	-0.0014(18)	-0.0097(15)	-0.0161(18)
C37	0.0341(19)	0.049(2)	0.035(2)	-0.0028(16)	-0.0107(14)	-0.0164(17)
C38	0.041(2)	0.059(2)	0.042(2)	-0.0151(18)	-0.0121(16)	-0.0179(19)
C39	0.047(2)	0.048(2)	0.050(2)	-0.0072(19)	-0.0150(17)	-0.0256(19)
C40	0.036(2)	0.053(2)	0.046(2)	-0.0009(18)	-0.0041(16)	-0.0227(18)
C41	0.0312(19)	0.045(2)	0.042(2)	-0.0093(17)	-0.0074(15)	-0.0111(16)
C42	0.041(2)	0.051(2)	0.067(3)	-0.018(2)	-0.0021(18)	-0.0253(19)
C43	0.034(2)	0.065(3)	0.054(2)	-0.025(2)	0.0060(16)	-0.0230(19)
C44	0.038(2)	0.046(2)	0.062(3)	-0.013(2)	-0.0095(18)	-0.0117(18)
C45	0.041(2)	0.077(3)	0.047(2)	-0.013(2)	-0.0165(17)	-0.018(2)
C46	0.041(2)	0.064(3)	0.087(3)	-0.043(2)	-0.015(2)	-0.018(2)
C47	0.0338(18)	0.0397(19)	0.039(2)	-0.0054(15)	-0.0001(14)	-0.0189(16)
C48	0.048(2)	0.037(2)	0.038(2)	-0.0047(16)	-0.0025(16)	-0.0201(18)
C49	0.084(3)	0.058(3)	0.042(2)	-0.004(2)	-0.016(2)	-0.023(2)
C50	0.132(5)	0.088(3)	0.041(3)	-0.001(2)	-0.001(3)	-0.053(3)
C51	0.040(2)	0.045(2)	0.045(2)	-0.0142(17)	-0.0033(16)	-0.0129(18)
C52	0.051(2)	0.044(2)	0.044(2)	-0.0165(17)	-0.0053(17)	-0.014(2)
C53	0.087(4)	0.067(3)	0.140(5)	-0.054(3)	-0.049(3)	-0.010(3)
C54	0.089(4)	0.116(5)	0.165(7)	-0.045(5)	-0.003(4)	-0.051(4)

==========

The Temperature Factor has the Form of Exp(-T) Where

T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

T = 2*(Pi**2)*Sumij(h(i)*h(j)*U(i,j)*Astar(i)*Astar(j)), for Anisotropic Atoms. Astar(i) are Reciprocal Axial Lengths and h(i) are the Reflection Indices.

Table S2-5. Hydrogen Atom Positions and Isotropic Displacement Parameters for **2b**

Atom	x	y	z	U(iso) [Ang^2]
H1A	0.93158	0.46024	0.14706	0.0426
H1B	0.88640	0.58830	0.15760	0.0426
H4	0.55513	0.49127	0.39547	0.0422
H5	0.70931	0.41583	0.46981	0.0451
H7	0.92183	0.42879	0.27624	0.0399
H11	1.13565	0.42974	0.49958	0.0647
H12	1.31646	0.28179	0.57637	0.0878
H13	1.33032	0.07339	0.60850	0.0921
H14	1.15852	0.08398	0.55296	0.0718
H15	0.88153	0.35873	0.64734	0.0664
H16	1.00046	0.45798	0.66311	0.0707
H17	1.17597	0.29653	0.73950	0.0772
H18	1.16752	0.09523	0.77136	0.0866
H19	0.98352	0.13431	0.71379	0.0842
H20A	0.37571	0.65840	0.24062	0.0452
H20B	0.42755	0.65578	0.31113	0.0452
H22A	0.39919	0.30466	0.41932	0.0710
H22B	0.29579	0.36365	0.36449	0.0710
H23A	0.40950	0.24960	0.28329	0.1468
H23B	0.41043	0.16376	0.36847	0.1468
H23C	0.51734	0.19578	0.33283	0.1468
H24A	0.49158	0.50929	0.17567	0.0437
H24B	0.62678	0.47032	0.16751	0.0437
H26A	0.57845	0.74174	-0.04720	0.0968
H26B	0.44529	0.76944	-0.02608	0.0968
H27A	0.60154	0.59843	-0.10284	0.1599
H27B	0.49912	0.71895	-0.14197	0.1599
H27C	0.47184	0.61659	-0.07734	0.1599
H28A	0.77844	0.66582	0.04313	0.0415
H28B	0.91459	0.61934	0.02609	0.0415
H31	0.84920	0.41519	-0.18347	0.0468
H32	0.83510	0.59804	-0.26790	0.0520
H34	0.82466	0.70806	-0.08687	0.0430
H38	0.76589	1.11317	-0.27615	0.0556
H39	0.80381	1.25637	-0.40456	0.0556
H40	0.88397	1.14455	-0.50688	0.0559
H41	0.89873	0.93179	-0.44421	0.0499
H42	0.55558	1.00779	-0.33456	0.0606
H43	0.50161	1.21518	-0.32455	0.0586
H44	0.54186	1.34444	-0.45905	0.0608
H45	0.62017	1.21723	-0.55375	0.0676
H46	0.62891	1.00685	-0.47547	0.0692

H47A	0.76251	0.27077	0.04618	0.0458
H47B	0.74854	0.39534	0.04771	0.0458
H49A	0.93128	0.22255	0.24925	0.0782
H49B	0.95081	0.09912	0.24135	0.0782
H50A	0.75711	0.24025	0.32015	0.1359
H50B	0.85395	0.11546	0.36031	0.1359
H50C	0.76796	0.12318	0.30787	0.1359
H51A	0.96036	0.16155	-0.02210	0.0539
H51B	0.96851	0.24399	-0.10710	0.0539
H53A	0.83447	0.00380	-0.13829	0.1109
H53B	0.72601	0.12052	-0.12795	0.1109
H54A	0.81791	-0.09295	-0.00983	0.1803
H54B	0.69610	-0.03851	-0.04390	0.1803
H54C	0.71802	0.02480	0.00580	0.1803

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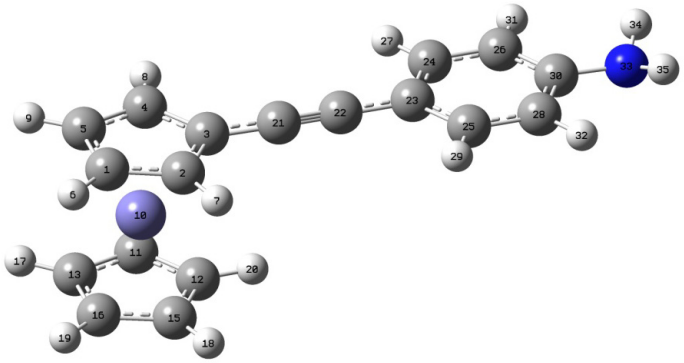
The Temperature Factor has the Form of Exp(-T) Where

T = 8*(Pi**2)*U*(Sin(Theta)/Lambda)**2 for Isotropic Atoms

VI- Computational details

V-1- Optimized geometry, three lower frequencies for ***II-A***

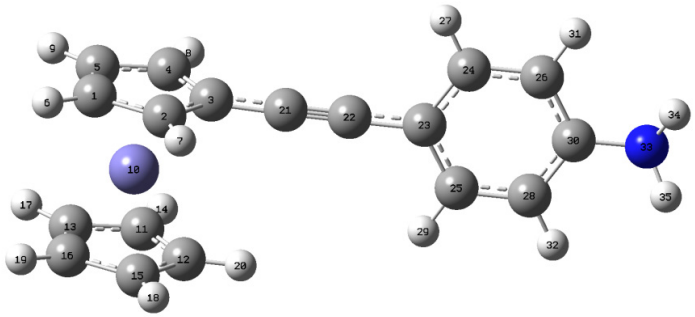


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.008235	-0.023242	0.000725
2	6	0	-0.003207	-0.011775	1.424637
3	6	0	1.365958	-0.005260	1.870204
4	6	0	2.195501	-0.028343	0.693752
5	6	0	1.346839	-0.033474	-0.449681
6	1	0	-0.888270	-0.056450	-0.629468
7	1	0	-0.868699	-0.023260	2.074377
8	1	0	3.277400	-0.055419	0.696122
9	1	0	1.674389	-0.076664	-1.480886
10	26	0	0.973624	-1.674523	0.729470
11	6	0	2.183802	-3.331865	0.739819
12	6	0	1.356570	-3.313196	1.902963
13	6	0	1.332680	-3.346765	-0.407359
14	1	0	3.266085	-3.298886	0.729270
15	6	0	-0.005569	-3.316063	1.476032
16	6	0	-0.020713	-3.337170	0.047710
17	1	0	1.656979	-3.329279	-1.440411
18	1	0	-0.873735	-3.270107	2.121617
19	1	0	-0.902852	-3.311916	-0.580059
20	1	0	1.701883	-3.243560	2.927044
21	6	0	1.812868	0.040532	3.213853
22	6	0	2.197035	0.096097	4.368982
23	6	0	2.642016	0.170740	5.717739
24	6	0	4.014095	0.157166	6.035298
25	6	0	1.724314	0.262497	6.782168
26	6	0	4.447857	0.233156	7.351410
27	1	0	4.742811	0.088571	5.232071
28	6	0	2.155925	0.338656	8.098875
29	1	0	0.659936	0.276447	6.563591
30	6	0	3.526723	0.327068	8.408613
31	1	0	5.514485	0.214991	7.567973
32	1	0	1.423977	0.403206	8.901985
33	7	0	3.958933	0.345856	9.731075
34	1	0	4.905446	0.670591	9.879662
35	1	0	3.312821	0.745453	10.399079

	1			2			3		
	A			A			A		
Frequencies --	18.5137			26.8140			31.6975		
Red. masses --	3.6948			6.0460			3.5927		
Frc consts --	0.0007			0.0026			0.0021		
IR Inten --	0.4836			0.8150			0.1086		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.05	-0.02	0.03	-0.04	-0.05	-0.07	-0.01	0.00	0.02
2 6	-0.04	-0.04	0.03	-0.03	0.04	-0.07	0.03	0.00	0.02
3 6	-0.04	-0.01	0.02	-0.03	0.10	-0.07	0.04	0.00	-0.01

4	6	-0.05	0.03	0.02	-0.04	0.05	-0.08	0.01	0.00	-0.04
5	6	-0.06	0.03	0.02	-0.04	-0.05	-0.07	-0.02	0.00	-0.01
6	1	-0.06	-0.03	0.04	-0.04	-0.12	-0.06	-0.03	0.00	0.05
7	1	-0.04	-0.08	0.04	-0.03	0.05	-0.07	0.04	0.01	0.05
8	1	-0.05	0.07	0.01	-0.03	0.08	-0.08	0.01	0.00	-0.07
9	1	-0.06	0.06	0.02	-0.04	-0.10	-0.07	-0.05	-0.01	-0.02
10	26	0.00	0.00	-0.01	0.01	0.02	0.04	0.01	0.00	0.00
11	6	0.05	0.03	-0.02	0.07	0.06	0.18	0.00	0.00	-0.19
12	6	0.04	-0.01	-0.03	0.05	0.12	0.17	0.19	0.00	-0.06
13	6	0.06	0.03	-0.03	0.08	-0.06	0.17	-0.18	0.00	-0.06
14	1	0.05	0.06	-0.01	0.06	0.09	0.19	0.00	-0.01	-0.37
15	6	0.04	-0.04	-0.05	0.06	0.05	0.15	0.12	0.00	0.16
16	6	0.06	-0.02	-0.05	0.07	-0.06	0.15	-0.11	0.00	0.16
17	1	0.07	0.06	-0.03	0.09	-0.13	0.17	-0.35	-0.01	-0.11
18	1	0.03	-0.08	-0.06	0.05	0.07	0.14	0.23	0.01	0.30
19	1	0.06	-0.03	-0.06	0.08	-0.14	0.14	-0.21	0.00	0.31
20	1	0.02	-0.02	-0.03	0.04	0.21	0.17	0.36	0.00	-0.12
21	6	-0.03	-0.02	0.02	-0.03	0.14	-0.08	0.06	0.01	-0.02
22	6	-0.02	-0.02	0.02	-0.03	0.13	-0.08	0.06	0.01	-0.02
23	6	-0.01	-0.01	0.01	-0.02	0.07	-0.08	0.03	0.00	-0.01
24	6	-0.01	-0.22	0.02	-0.02	-0.02	-0.07	0.02	-0.02	0.03
25	6	0.00	0.22	0.01	-0.02	0.06	-0.07	0.00	0.03	-0.04
26	6	0.00	-0.21	0.01	-0.02	-0.12	-0.07	-0.02	-0.03	0.04
27	1	-0.02	-0.40	0.02	-0.03	-0.01	-0.08	0.04	-0.04	0.05
28	6	0.01	0.23	0.00	-0.02	-0.04	-0.07	-0.04	0.02	-0.03
29	1	0.01	0.39	0.00	-0.02	0.13	-0.07	0.00	0.05	-0.07
30	6	0.01	0.02	0.00	-0.02	-0.14	-0.07	-0.05	0.00	0.02
31	1	-0.01	-0.38	0.01	-0.02	-0.19	-0.07	-0.03	-0.05	0.08
32	1	0.02	0.41	0.00	-0.02	-0.05	-0.06	-0.07	0.04	-0.05
33	7	0.01	0.03	0.00	-0.02	-0.26	-0.06	-0.09	-0.01	0.03
34	1	0.07	-0.13	-0.02	0.00	-0.32	-0.04	-0.09	-0.03	0.06
35	1	0.08	0.19	-0.03	0.00	-0.27	-0.04	-0.11	0.01	0.01

V-2- Optimized geometry, three lower frequencies for ***II-B***



Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002344	-0.000000396	0.000001203
2	6	-0.000001796	-0.000001826	0.000001684
3	6	-0.000001591	-0.000000102	0.000001957
4	6	-0.000002294	0.000002572	-0.000000166
5	6	-0.000001608	0.000002361	0.000002115
6	1	-0.000002121	-0.000001425	0.000001088
7	1	-0.000001725	-0.000003184	0.000001047
8	1	-0.000001892	0.000004027	0.000000322
9	1	-0.000002347	0.000002929	0.000000626
10	26	0.000000308	0.000000583	-0.000001209
11	6	0.000003454	0.000002414	-0.000000832
12	6	0.000003337	-0.000000048	-0.000002267
13	6	0.000002635	0.000002297	-0.000002874
14	1	0.000003103	0.000003955	-0.000002136
15	6	0.000003362	-0.000001594	-0.000001715
16	6	0.000003208	-0.000000548	-0.000001246
17	1	0.000002472	0.000002910	-0.000001663
18	1	0.000003440	-0.000003232	-0.000001040
19	1	0.000002745	-0.000001478	-0.000001048
20	1	0.000003711	0.000000349	-0.000001653
21	6	-0.000001552	0.000000241	0.000000552
22	6	-0.000001254	-0.000000153	0.000000747
23	6	-0.000001097	-0.000000535	0.000000479
24	6	-0.000002659	-0.000000397	0.000001252
25	6	0.000000579	-0.000000561	-0.000000197
26	6	-0.000002688	-0.000000717	0.000001330
27	1	-0.000004387	-0.000000305	0.000002031
28	6	0.000000991	-0.000000826	-0.000000273
29	1	0.000002185	-0.000000551	-0.000000939
30	6	-0.000000803	-0.000000825	0.000000414
31	1	-0.000004114	-0.000000710	0.000001974
32	1	0.000002504	-0.000000949	-0.000000999
33	7	-0.000000627	-0.000000978	0.000000486
34	1	-0.000001863	-0.000001594	0.000001044
35	1	0.000000727	-0.000001705	-0.000000093

	1			2			3		
	A			A			A		
Frequencies --	-12.8153			27.7328			30.4596		
Red. masses --	3.7021			5.7032			3.6504		
Frc consts --	0.0004			0.0026			0.0020		
IR Inten --	0.4134			0.6187			0.2066		
Atom AN	X	Y	Z	X	Y	Z	X	Y	Z
1 6	-0.05	-0.03	0.02	-0.02	-0.05	-0.08	-0.01	-0.01	0.00
2 6	-0.05	-0.04	0.02	-0.03	0.04	-0.08	0.03	0.01	0.00
3 6	-0.04	0.00	0.01	-0.04	0.09	-0.07	0.04	0.02	-0.03
4 6	-0.05	0.04	0.01	-0.02	0.04	-0.06	0.01	0.00	-0.04
5 6	-0.05	0.02	0.01	-0.01	-0.05	-0.07	-0.02	-0.01	-0.03
6 1	-0.05	-0.05	0.02	-0.01	-0.11	-0.09	-0.02	-0.01	0.02
7 1	-0.04	-0.07	0.02	-0.04	0.06	-0.09	0.04	0.02	0.02
8 1	-0.05	0.07	0.00	-0.02	0.06	-0.04	0.01	0.00	-0.07
9 1	-0.06	0.04	0.01	0.00	-0.11	-0.06	-0.04	-0.03	-0.03
10 26	0.00	0.00	0.00	0.01	0.02	0.04	0.01	0.00	0.00

11	6	0.06	0.04	-0.01	0.05	0.04	0.21	0.01	0.00	-0.17
12	6	0.06	0.00	-0.01	0.00	0.11	0.18	0.20	0.02	-0.03
13	6	0.06	0.02	-0.01	0.10	-0.06	0.18	-0.18	-0.01	-0.03
14	1	0.06	0.07	-0.01	0.05	0.07	0.25	0.01	0.00	-0.35
15	6	0.06	-0.04	-0.02	0.02	0.05	0.12	0.13	0.01	0.19
16	6	0.06	-0.03	-0.02	0.08	-0.06	0.12	-0.11	-0.01	0.19
17	1	0.06	0.04	-0.01	0.14	-0.13	0.19	-0.35	-0.03	-0.09
18	1	0.05	-0.07	-0.02	-0.01	0.08	0.08	0.23	0.02	0.33
19	1	0.06	-0.05	-0.02	0.10	-0.13	0.08	-0.21	-0.01	0.33
20	1	0.05	0.00	-0.01	-0.04	0.20	0.18	0.36	0.03	-0.09
21	6	-0.04	0.01	0.01	-0.05	0.13	-0.07	0.05	0.02	-0.03
22	6	-0.03	0.01	0.01	-0.05	0.13	-0.07	0.05	0.02	-0.03
23	6	-0.02	0.01	0.01	-0.04	0.06	-0.06	0.02	0.01	-0.02
24	6	0.20	0.00	-0.07	-0.02	0.02	0.01	0.02	0.00	-0.01
25	6	-0.23	0.01	0.07	-0.04	0.01	-0.14	-0.01	0.00	-0.02
26	6	0.22	-0.01	-0.07	0.00	-0.07	0.01	-0.02	-0.01	0.01
27	1	0.36	-0.01	-0.12	-0.02	0.06	0.07	0.05	0.01	0.00
28	6	-0.21	0.00	0.07	-0.02	-0.08	-0.14	-0.05	-0.01	-0.01
29	1	-0.40	0.02	0.13	-0.06	0.04	-0.20	-0.01	0.01	-0.04
30	6	0.01	0.00	-0.01	0.00	-0.12	-0.07	-0.06	-0.02	0.01
31	1	0.39	-0.02	-0.13	0.01	-0.10	0.07	-0.02	-0.02	0.02
32	1	-0.37	0.01	0.12	-0.02	-0.12	-0.21	-0.08	-0.02	-0.01
33	7	0.03	-0.02	-0.01	0.02	-0.21	-0.07	-0.10	-0.04	0.02
34	1	0.19	0.04	-0.06	0.04	-0.24	-0.01	-0.11	-0.04	0.03
35	1	-0.12	0.05	0.04	0.03	-0.25	-0.12	-0.13	-0.04	0.01

VII- References

(1) Tsien, R. Y. *Biochemistry* **1980**, *19*, 2396.
(2) Grynkiewicz, G.; Poenie, M.; Tsien, R. Y. *J. Biol. Chem.* **1985**, *260*, 3440.
(3) Tsien, R.; Pozzan, T. *Methods Enzymol.* **1989**, *172*, 230.